CALIFORNIA STATE SCIENCE FAIR
2015 PROJECT SUMMARY

Name(s)
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Project Number
35256

Project Title

Biological Electron-Transfer Dynamics in Multiheme Cytochrome Complexes

Abstract

Objectives/Goals

Electron transfer (ET) governs all known energy-conversion processes in biology. A remarkable example is the recent discovery of rapid ET along electrically conducting bacterial nanowires produced by the bacteria Shewanella oneidensis MR-1. The outer-membrane cytochrome, MtrF and OmcA, are hypothesized media for ET, but how these multiheme cytochromes are assembled into a conducting complex remains a mystery. Thus, the goal of my project was to determine the structure of the MtrF-OmcA complex and visualize ET dynamics in it to better understand the underlying electric conduction mechanisms.

Methods/Materials

Here, I determine the structure of the MtrF-OmcA complex and study ET dynamics in it by combining the use of a homology modeling server, protein docking software, kinetic Monte Carlo (KMC) simulation, and visualization. I developed a computational framework including the entire workflow. In particular, I developed a C-RANK program to screen complexes according to biological plausibility as well as a plugin to the Visual Molecular Dynamics software named ETViz to animate ET dynamics.

Results

My visual simulation results reveal novel nonequilibrium phase transitions with which Shewanella efficiently responds to a change in its electrochemical environment. The KMC results, when compared with experimentally observed respiration rates, suggest that life operates around the triple phase junction.

Conclusions/Discussion

My simulation and visualization results shed useful light on boosting the efficiency of Shewanella-based microbial fuel cells by increasing the ET rate toward solving the global energy problem. Currently, I am working on a larger study of ET mechanisms along a lattice of outer-membrane cytochrome complexes on the entire bacterial nanowire.

Summary Statement

I developed an electron transfer visualization software to reveal novel nonequilibrium phase transitions with which a bacterium efficiently responds to a change in its electrochemical environment.

Help Received

Research Supervised by Prof. Mohamed Y. El-Naggar (USC) and Prof. Tao Wei (Lamar University)